

# Persistent Currents in the Heisenberg chain with a weak link

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(February 1, 2008)

## Abstract

The Heisenberg chain with a weak link is studied, as a simple example of a quantum ring with a constriction or defect. The Heisenberg chain is equivalent to a spinless electron gas under a Jordan-Wigner transformation. Using density matrix renormalization group and quantum Monte Carlo methods we calculate the spin/charge stiffness of the model, which determines the strength of the ‘persistent currents’. The stiffness is found to scale to zero in the weak link case, in agreement with renormalization group arguments of Eggert and Affleck, and Kane and Fisher.

PACS Indices: 73.23.Ra, 75.10.Jm, 68.66.La

## I. INTRODUCTION

Technological advances in recent years have allowed the fabrication of electrical and even mechanical devices on the nanometer scale, where individual atoms or electrons can be manipulated. The physics of these devices poses a plethora of fundamental questions through a rich variety of novel quantum effects [1]. This has led to an upsurge of theoretical interest in the physics of ‘quantum wires’, ‘quantum dots’ and more general physics at the mesoscopic or nanometer scale [2]. The effects of electron-electron interactions are typically enhanced in systems of reduced dimensionality, leading to nonperturbative effects, such as the breakdown of Fermi liquid behavior in one-dimensional metals, and single-electron charging effects in quasi-zero-dimensional systems (quantum dots). An important milestone in the nascent field of nanomechanics was the experimental discovery that not only the electrical but also the *mechanical* properties of metallic structures on the nanometer scale exhibit apparently universal nonmonotonic quantum corrections [3,4], which could be explained theoretically within the framework of a Jellium model [5].

In the electrical domain, paradigm systems to investigate mesoscopic behavior have long been small ring-shaped or multiply connected devices, where the application of a magnetic flux piercing the device leads to persistent currents. However, the theoretical prediction of these persistent currents, first in superconducting and then in normal conducting materials, has always predated experimental investigation, which has only become feasible in the last decade [6]. Very recently, with the discovery of a tunable Kondo effect in quantum dots, the persistent currents of multiply connected systems with magnetic quantum dots - Kondo rings for short - have aroused considerable interest [7–9].

In this paper we explore a very simple system, which may serve to model a metallic quantum wire ring with a weak junction, or *constriction*. It consists of the standard spin-1/2 Heisenberg antiferromagnetic spin chain, which by a Jordan-Wigner transformation is equivalent to a spinless electron gas in one dimension, where the exchange coupling is weakened at a single link. We use Density Matrix Renormalization Group (DMRG) [10,11] and Quantum Monte Carlo (QMC) methods [12] to obtain numerical results on chains of up to 256 sites, and perform finite-size scaling extrapolations to the bulk limit. We study the spin stiffness, which under the Jordan-Wigner transformation is equivalent to the charge stiffness of the electron gas and is related to the persistent current, as a function of the weak link coupling. We also study the spin correlations across the weak link.

Eggert and Affleck [13] have previously studied the Heisenberg chain with an isolated impurity using exact diagonalization and conformal field theory techniques. They find that in renormalization group language a single weak link across the ends of an open chain corresponds to an irrelevant operator, and therefore the open chain is a stable fixed point under such a perturbation. Thus they predict that in the bulk limit a chain with a weak link will behave like an open chain. These findings for a concrete model system are in agreement with the general predictions of Kane and Fisher [14] for the general one-dimensional interacting electron gas, i.e. the Luttinger liquid. An integrable version of the Heisenberg spin chain with defects has also been studied [15–17]. The case of a single defect corresponds to a weak link. However, as opposed to the case discussed here where only one bond is modified, integrability requires a modification of two adjacent bonds and an additional three-spin coupling. Although the defect of this integrable chain is completely transparent to particle

scattering, the persistent current is renormalized by the defect strength.

Let us briefly review [18] how the persistent current arises, for the simple case of free electrons. Start from the real-space continuum Hamiltonian

$$H = -\frac{\hbar^2}{2m_e} \sum_{\alpha} \int_0^L dx \psi_{\alpha}^{\dagger}(x) \partial_x^2 \psi_{\alpha}(x) \quad (1)$$

where  $\psi_{\alpha}(x)$  is an electron field with spin index  $\alpha = \pm 1$ , and  $L$  is the circumference of the ring. Now thread the ring with a magnetic flux  $\Phi$ , producing an Aharonov-Bohm effect [19]. The quantum phase

$$\frac{e}{\hbar c} \int_0^L A_{\mu} d_{\mu} x = \frac{e}{\hbar c} \Phi \quad (2)$$

can be encoded via a gauge transformation in the twisted boundary conditions

$$\psi_{\alpha}(L) = e^{i\phi} \psi_{\alpha}(0), \quad (3)$$

where

$$\phi = 2\pi \frac{\Phi}{\Phi_0} \quad (4)$$

and  $\Phi_0 = hc/e$  is the elementary flux quantum.

When an Aharonov-Bohm field is applied, the Hamiltonian acquires the usual interaction term (we set  $\hbar = c = 1$  henceforth)

$$H_{int} = - \int dx A_{\mu} J^{\mu}(x). \quad (5)$$

Thus for a constant field  $A_1 = \Phi/L$  the corresponding “persistent current” is given by the Feynman-Hellman theorem:

$$J^1 \equiv I(\Phi) = - \frac{\partial E_0}{\partial \Phi} \quad (6)$$

which can be expanded

$$I(\Phi) = -D_c \frac{\Phi}{L} + O\left(\left(\frac{\Phi}{L}\right)^2\right) \quad (7)$$

where  $D_c$  is the “charge stiffness”. If we *assume* that  $I(\Phi)$  is purely linear in  $\Phi$  (as can be proved for the pure Heisenberg chain [20]), then the charge stiffness and hence the persistent current can be estimated from the difference in energy between the system with anti-periodic boundary conditions ( $E_0^- = E_0(\Phi = \Phi_0/2)$ ) and periodic boundary conditions ( $(E_0^+ = E_0(\Phi = 0))$ )

$$D_c = \frac{8L}{\Phi_0^2} [E_0^- - E_0^+] \quad (8)$$

The corresponding quantity in the Heisenberg chain is the spin stiffness.

In section II of the paper we briefly summarize the DMRG and QMC methods used to calculate this quantity. In section III we present our results, and in section IV our conclusions are summarized.

## II. METHOD

We study the spin-1/2 Heisenberg quantum spin chain with a single weak coupling  $J' < J$  between two adjacent spins located between sites  $i = N$  and  $i = 1$ . The Hamiltonian is

$$H = J \sum_{i=1}^{N-1} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J' \mathbf{S}_N \cdot \mathbf{S}_1. \quad (9)$$

There are a total of  $N$  sites in the ring. We study  $J'/J$  in the range  $[0, 1]$ , hence we have either open or periodic boundary conditions (OBC or PBC) at the extremities of this range. We also consider anti-periodic boundary conditions in the same range of  $J'/J$ , to obtain the charge stiffness  $D_c$  according to (8). The model in these limits is exactly solvable by Bethe ansatz [21], and hence is often used as a testing ground for various DMRG methods [10,22]. The quantities that have been calculated using DMRG include the ground state energy, the singlet and triplet gaps, and correlation functions.

The “infinite-lattice” DMRG method [10] is used here, applied with periodic boundary conditions. The lattice is split into two blocks and two sites as shown in Fig. 1. The weak link is placed between block 1 and site 2. At any time the superblock consists of a system block and an environment block, plus two extra sites. The presence of the weak link destroys the translational invariance normally exploited in usual DMRG schemes, hence we cannot simply make a copy of the density matrix in one block and transfer it to the other block. Therefore in a single DMRG iteration, two density matrices are constructed (one for each block), and the basis set for each block originates from its corresponding density matrix. Each block increases in size by a single site in a single DMRG iteration. We calculate results for lattice sizes  $N = 4$  to 64, in steps of two. The quantities calculated here are the ground state energies, and the correlation of the spins across the weak link. The total number of density matrix eigenstates retained in a block was  $m = 350$  in the basis truncation procedure.

We also carried out quantum Monte Carlo simulations using the stochastic series expansion (SSE) method [12]. In this case, the spin stiffness can be directly calculated as the second derivative of the energy with respect to the phase, which is given in terms of the fluctuation of the winding number in the simulations [23].

## III. RESULTS

To estimate the accuracy of the DMRG, we perform convergence tests with  $m$ , the number of basis states retained in a block. Table I shows sample results for  $J'/J = 0.5$  and  $N = 64$  with both periodic and anti-periodic boundary conditions. We see good convergence with the number of basis states retained: in particular, for the ground state energy we have convergence to 1 part in  $10^6$ . We obtained independent estimates using SSE techniques for the periodic case, which yields  $E_0/J = -28.2178(3)$ , agreeing perfectly with the DMRG results. The correlations between the spins across the links have a marginally lower accuracy because of round-off error, but even here we have an error in the region of 1 part in  $10^4$ .

Since the SSE method is a finite-temperature quantum Monte Carlo method we have to run the simulations at sufficiently low temperature to converge the quantities of interest to their ground state values. In Table II we show the convergence of the energy and the

charge stiffness for a 256-site chain. All SSE results discussed below were obtained at inverse temperatures  $\beta$  where the results do not differ, within statistical errors, from results at  $\beta/2$ .

Ground state energies were calculated for the periodic and anti-periodic rings, as a function of the weak link coupling  $J'/J$ . Figs. 2 and 3 shows DMRG estimates for the quantity  $\Delta E_N = (E_0(N; J') - E_0(N; J' = J))/J$  as a function of  $J'/J$ , for several different lattice sizes up to  $N = 64$ . An extrapolation in  $1/N$  can be performed to extract the bulk limit for each value of  $J'$  by a simple polynomial fit to the data, giving us the extrapolated curve for the periodic and anti-periodic cases. It can be seen that for the periodic case the bulk values are approached from above, while for the anti-periodic case the limit is approached from below.

Putting together both the periodic and anti-periodic results for the energy, we can calculate the spin stiffness factor, given by

$$\rho_s = \frac{2N}{\pi^2 J} (E_0(N; \text{anti-periodic}) - E_0(N; \text{periodic})) \quad (10)$$

The results are shown in Fig. 4. At couplings other than  $J'/J = 1$  the values trend steadily down towards zero as the lattice size  $N$  increases. There is a marked difference in behavior for the isotropic case  $J'/J = 1$ , as the strong curvature towards zero is not apparent. One would naively expect to obtain a bulk limit by a simple linear extrapolation procedure, but in fact the work of Woynarovich and Eckle [24] has shown that there are logarithmic corrections to the ground state energy, and hence the stiffness. We can see the effects of these corrections for the  $J'/J = 1$  case, as there exists an exact result obtained by Hamer, Quispel and Batchelor [20] (equation (3.37) of ref. [20] with  $\gamma = 0$ )

$$\rho_s = \frac{1}{4}. \quad (11)$$

This does not seem in accord with the data in Fig 4, which appear to be approaching 0.27. A late, logarithmic downturn must therefore occur at very large lattice sizes.

Using field theoretical methods, Eggert and Affleck [13] have predicted that a chain with  $J' < J$  should be similar to an open chain (i.e.,  $J'/J = 0$ ). This implies that the spin [charge] stiffness should vanish as the system size  $N \rightarrow \infty$ . Fig. 5 shows SSE results [25] for the stiffness versus the system size ( $N = 16, 32, 64, 128$  and  $256$ ) for several values of  $J' \leq J$ . The results are in accordance with a scaling behavior

$$\rho_N(x) \sim a(x) N^{-\sigma} \quad (12)$$

where  $x = J'/J$ , and the index  $\sigma \simeq 2/3$ . Fig. 6 demonstrates that the data for large  $N$  can be well described, in fact, by a simple scaling form

$$\rho_N(x) \sim \frac{2.6x}{(1-x)} N^{-2/3}, \quad N \rightarrow \infty. \quad (13)$$

It is likely, however, that the true asymptotic correction-to-scaling behavior is again being disguised by logarithmic corrections.

We have also calculated the value of the spin correlation function across the weak link, i.e.  $\langle S_N^z S_1^z \rangle$ . Fig. 7 shows the behavior versus  $1/N^2$  for various values of  $J'/J$ . It can

be seen that the finite-lattice values generally approach a finite value in the bulk limit, as one would expect, except for the special case  $J'/J = 0$  where the link is open. Theoretical expectations [26] are that the correlation function should approach its bulk limit like  $1/N^2$ , up to logarithmic corrections.

The presence of a finite correlation across the weak link is just what one would naively expect when the weak-link coupling  $J'$  is non-zero. On the other hand, it might appear to contradict the previous statement that a chain with a weak link should renormalize to the open chain. The point here is that the weak-link correlation is a *local* quantity, not a bulk property. It is only bulk properties such as the spin-stiffness which scale to the value of the open chain.

#### IV. CONCLUSIONS

In summary, we have performed a finite-lattice study of the Heisenberg ring with a weak link, using both DMRG and QMC calculations on rings of up to 256 sites. The spin or ‘charge’ stiffness has been calculated either directly (QMC), or from the energy difference between the system with anti-periodic boundary conditions and that with periodic boundaries, assuming a quadratic dependence of the energy on the twist parameter  $\phi$  (DMRG).

The stiffness, and hence the persistent current, is found to scale to zero in the bulk limit  $N \rightarrow \infty$ , for any  $J' < J$ . This agrees with the renormalization group prediction of Eggert and Affleck [13], that the stable fixed point for this system corresponds to an open chain, so that the chain with a weak link will behave like an open chain, as regards its bulk properties.

We have also measured the spin-spin correlation across the weak link. A finite antiferromagnetic correlation remains in the bulk limit, depending on the coupling  $J'$  as one would expect. The renormalization group argument does not apply to a ‘local’ quantity such as this.

The asymptotic scaling behavior of these quantities has been disguised to some extent by logarithmic finite-size scaling corrections. Eggert and Affleck [13] have circumvented this problem by studying a modified model with an extra marginal operator; but we have not found this necessary for our present purposes.

For the future, it would be of interest to see how the results generalize to more complicated and interesting cases, such as higher spin chains, or real electronic models, such as the Hubbard model or its variant, the so-called  $t - J$  model. Another interesting extension of the present study would be to interpret the weak link and hence the modified bond in our model as caused by a mechanical force on a quantum wire. It would be interesting to see what conclusions could be drawn from our simple one-dimensional model for such a scenario.

#### V. ACKNOWLEDGEMENTS

We would like to thank Prof. I. Affleck for very useful correspondence. This work was supported by a grant from the Australian Research Council, and H.-P.E. was supported by an ARC-IREX Exchange Fellowship. A.W.S. was supported by the Academy of Finland (project 26175), and would also like to thank the School of Physics at UNSW for financial support through a Gordon Godfrey visitor fellowship. We are grateful for the computing

resources provided by the Australian Centre for Advanced Computing and Communications (ac3) and the Australian Partnership for Advanced Computing (APAC) National Facility.

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# TABLES

TABLE I. DMRG estimates of the ground state energy  $E_0/J$  and correlation  $\langle S_N^z S_1^z \rangle$  for  $N = 64$  sites at  $J'/J = 0.5$  as a function of  $m$ , the number of states retained per block. A SSE estimate of  $E_0/J = -28.2178(3)$  for PBC agrees very well with the DMRG data: here our final DMRG estimate is  $-28.21797(1)$ . The correlation between spins across the weak link also converges to better than 1 part in  $10^4$ . The anti-periodic boundary conditions yield similar levels of accuracy.

$m$	Periodic		Anti-periodic	
	$E_0/J$	$\langle S_N^z S_1^z \rangle$	$E_0/J$	$\langle S_N^z S_1^z \rangle$
96	-28.217652	-0.060888	-28.212779	-0.0560186
164	-28.217938	-0.061194	-28.213082	-0.0562742
234	-28.217964	-0.061219	-28.213123	-0.0563028
342	-28.217970	-0.061222	-28.213132	-0.0563091

TABLE II. The internal energy and the spin stiffness calculated in SSE simulations for a 256-site chain with  $J'/J = 1/4$  at different inverse temperatures  $\beta = J/T$ .

$\beta$	$E_0/NJ$	$\rho_s$
32	-0.44211(2)	0.0000(0)
64	-0.44237(1)	0.0008(1)
128	-0.442429(9)	0.0088(3)
256	-0.442443(5)	0.0202(5)
512	-0.442443(4)	0.0212(4)
1024	-0.442453(3)	0.0215(2)
2048	-0.442448(3)	0.0218(2)

# FIGURES

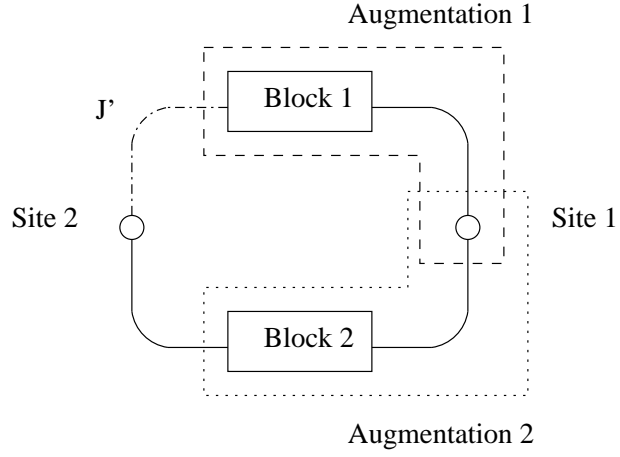


FIG. 1. The augmentation process within one DMRG iteration. Augmentation 1 (Augmentation 2) gives the new Block 1 (Block 2) in the next DMRG iteration.

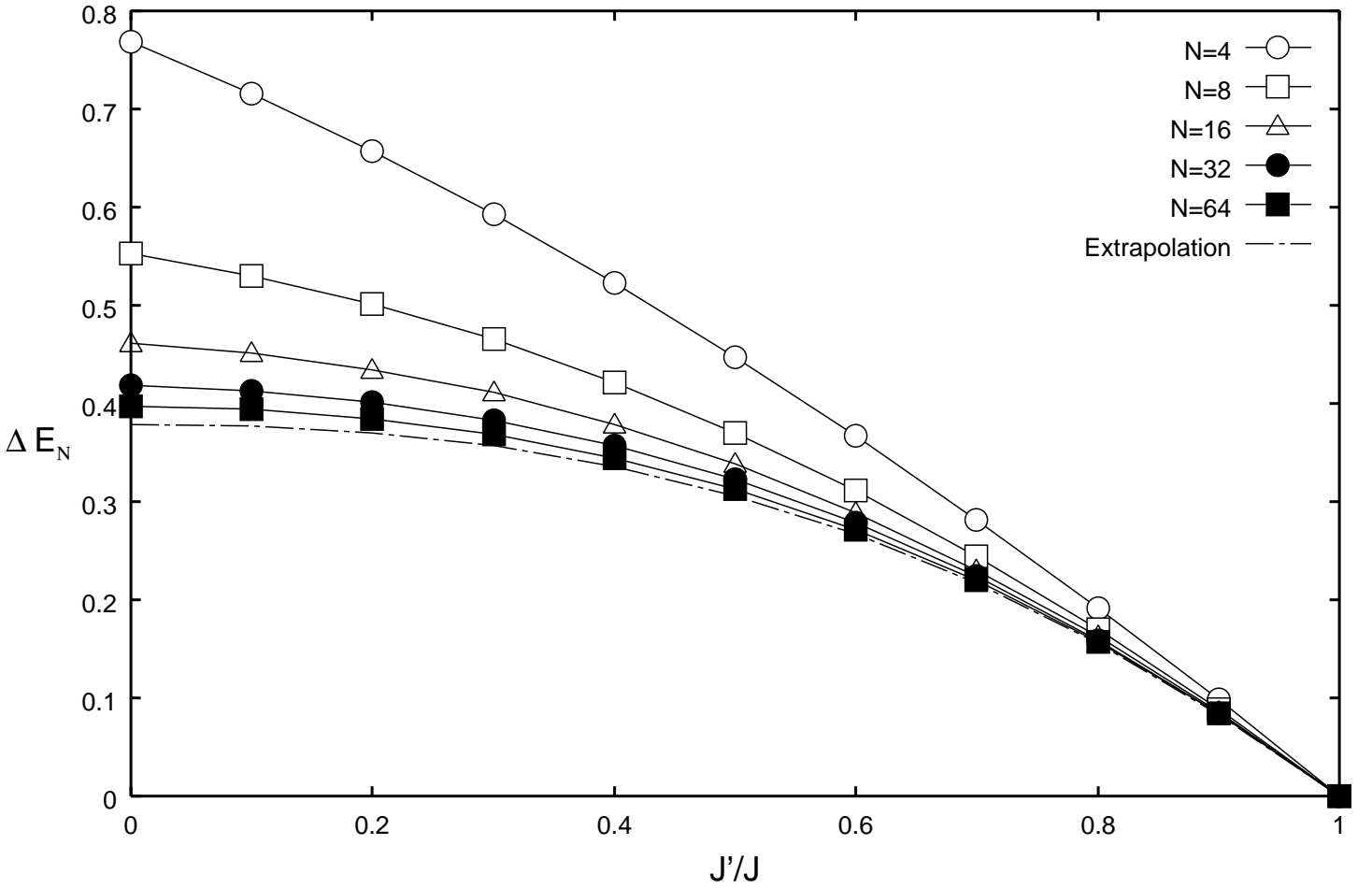


FIG. 2.  $\Delta E_N = (E_0(N; J') - E_0(N; J' = J))/J$  as a function of  $J'/J$  for the ring with periodic boundary conditions. The data is extrapolated using a simple fit to obtain the bulk limit.

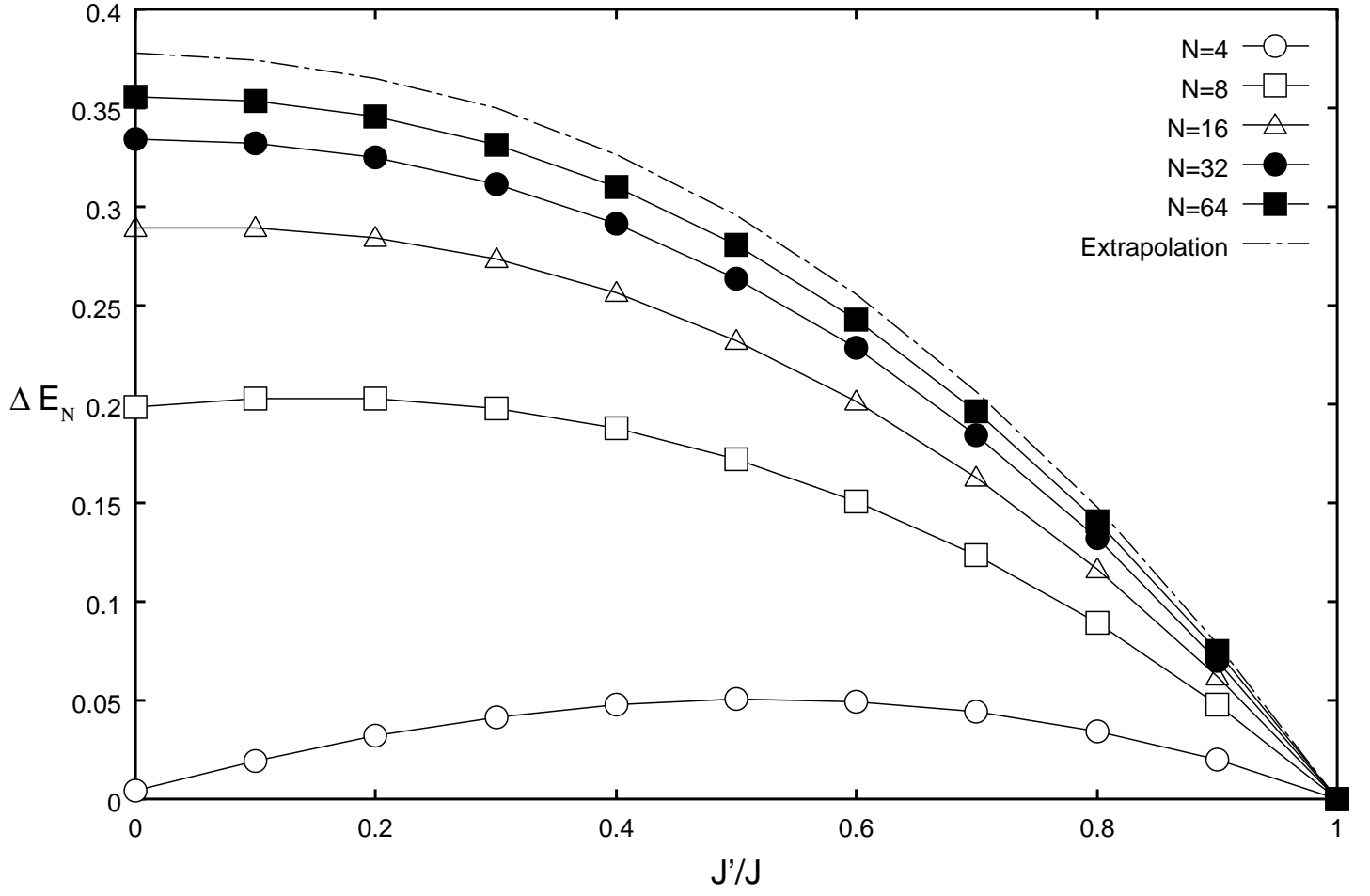


FIG. 3. As for Fig. 2, but with anti-periodic boundary conditions.

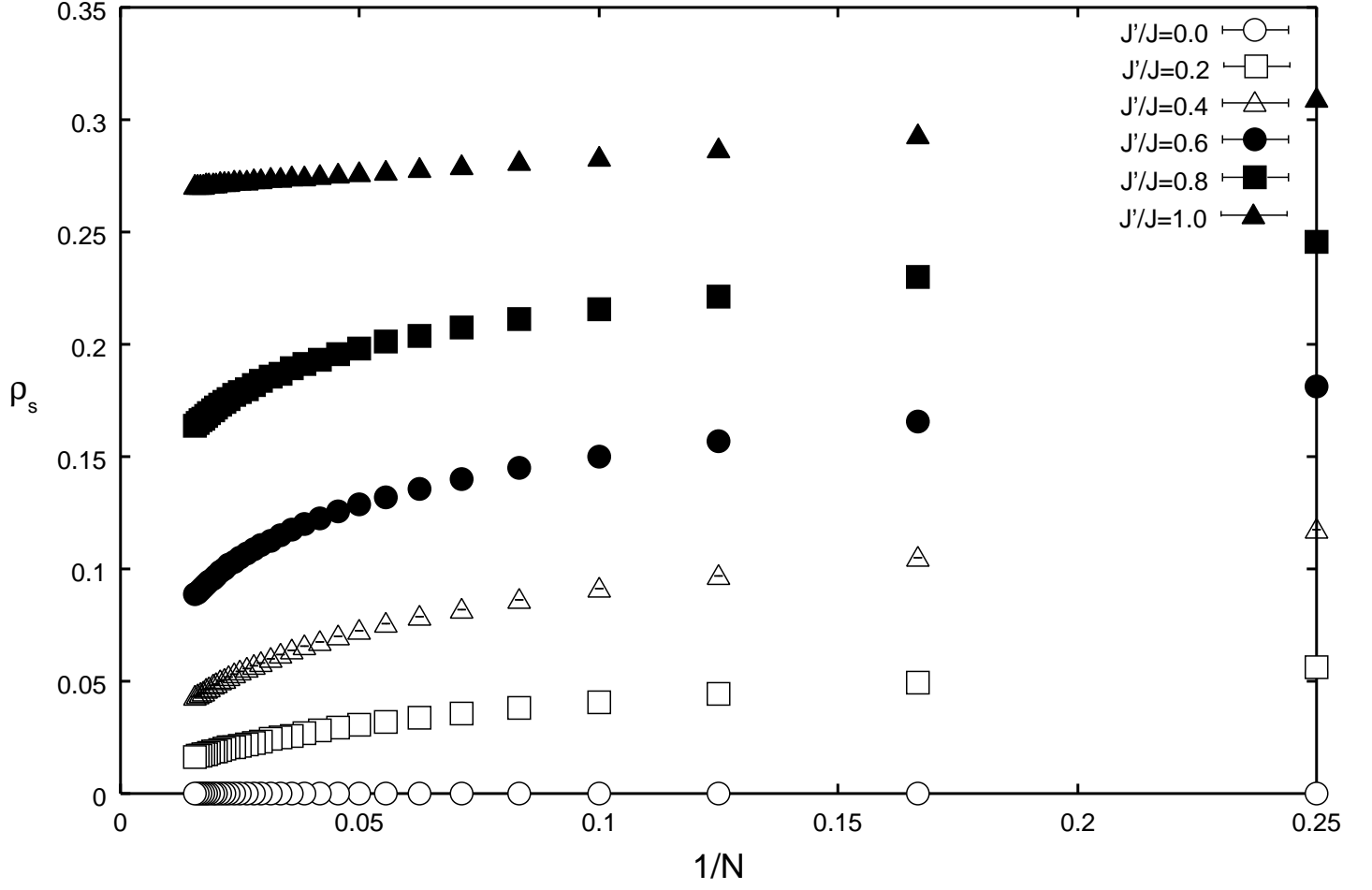


FIG. 4. The stiffness factor  $\rho_s$  as a function of  $1/N$ , for lattice sizes  $N = 4$  to  $64$ .

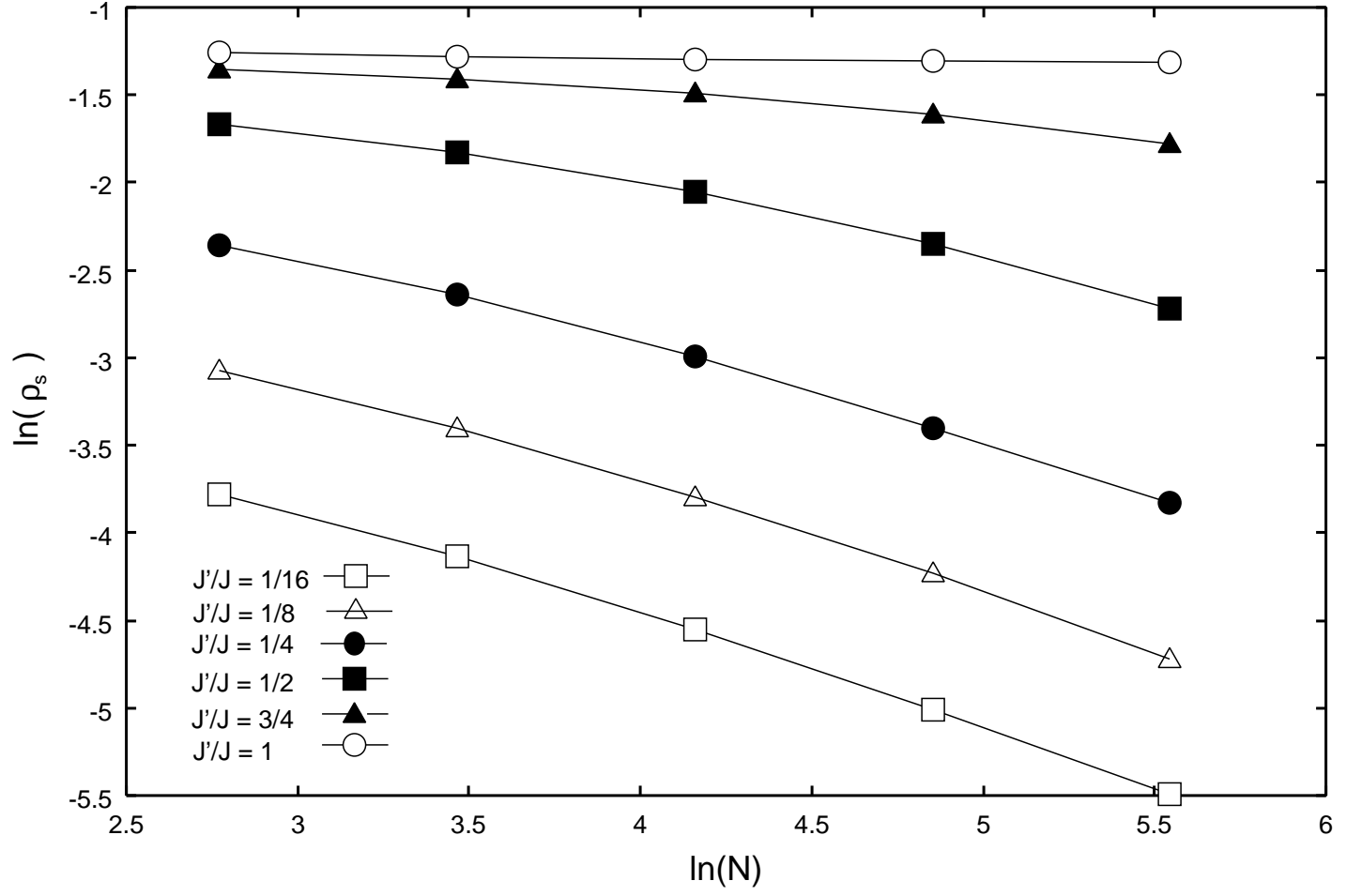


FIG. 5. SSE results for the stiffness factor  $\rho_s$  versus lattice sizes ( $N = 16, 32, 64, 128, 256$ ).

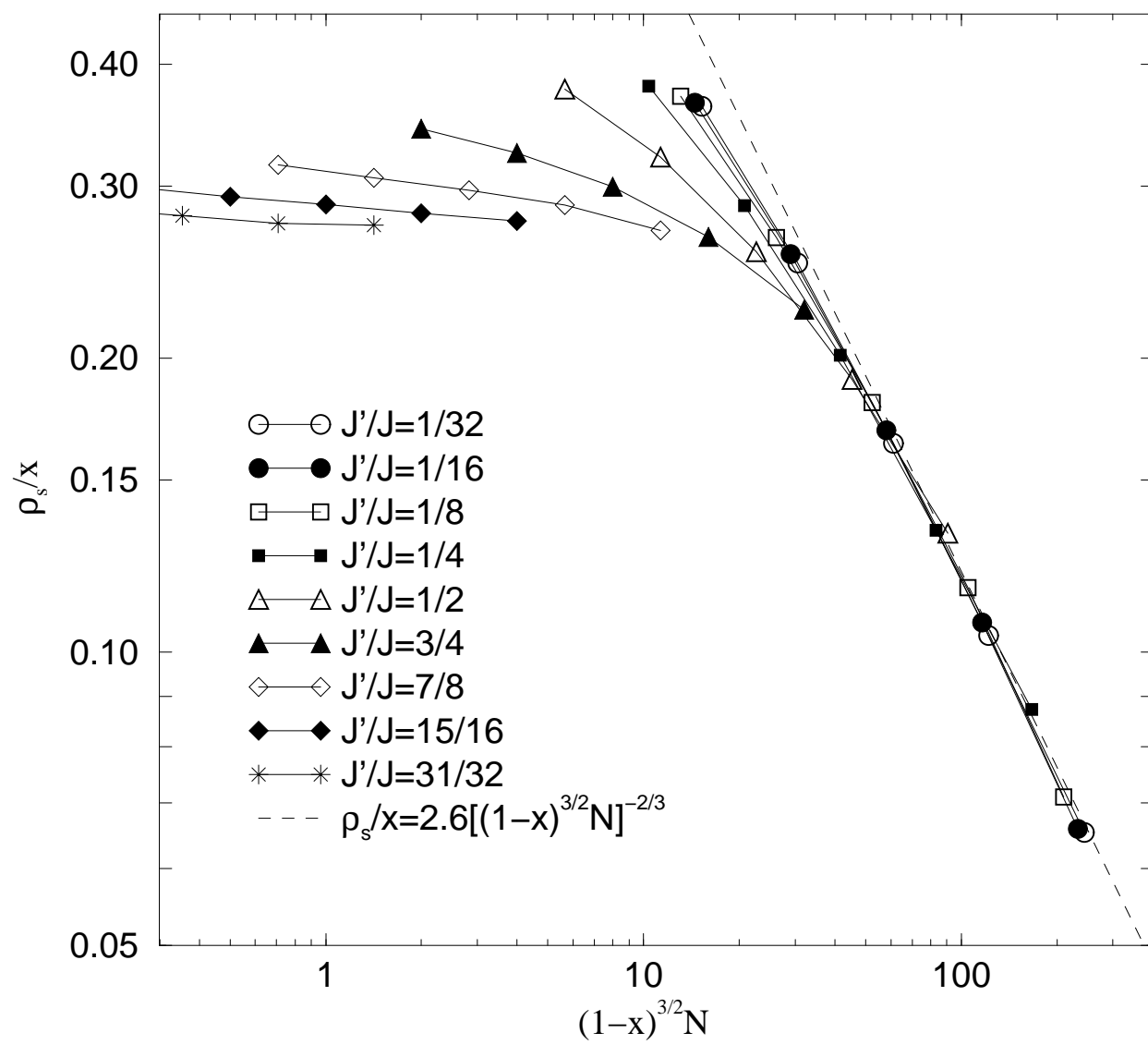


FIG. 6. Scaling plot of  $\rho_s/x$  versus  $(1-x)^{3/2}N$ , where  $x = J'/J$ . Also shown is the scaling form (13), which agrees with the data for large  $N$ .

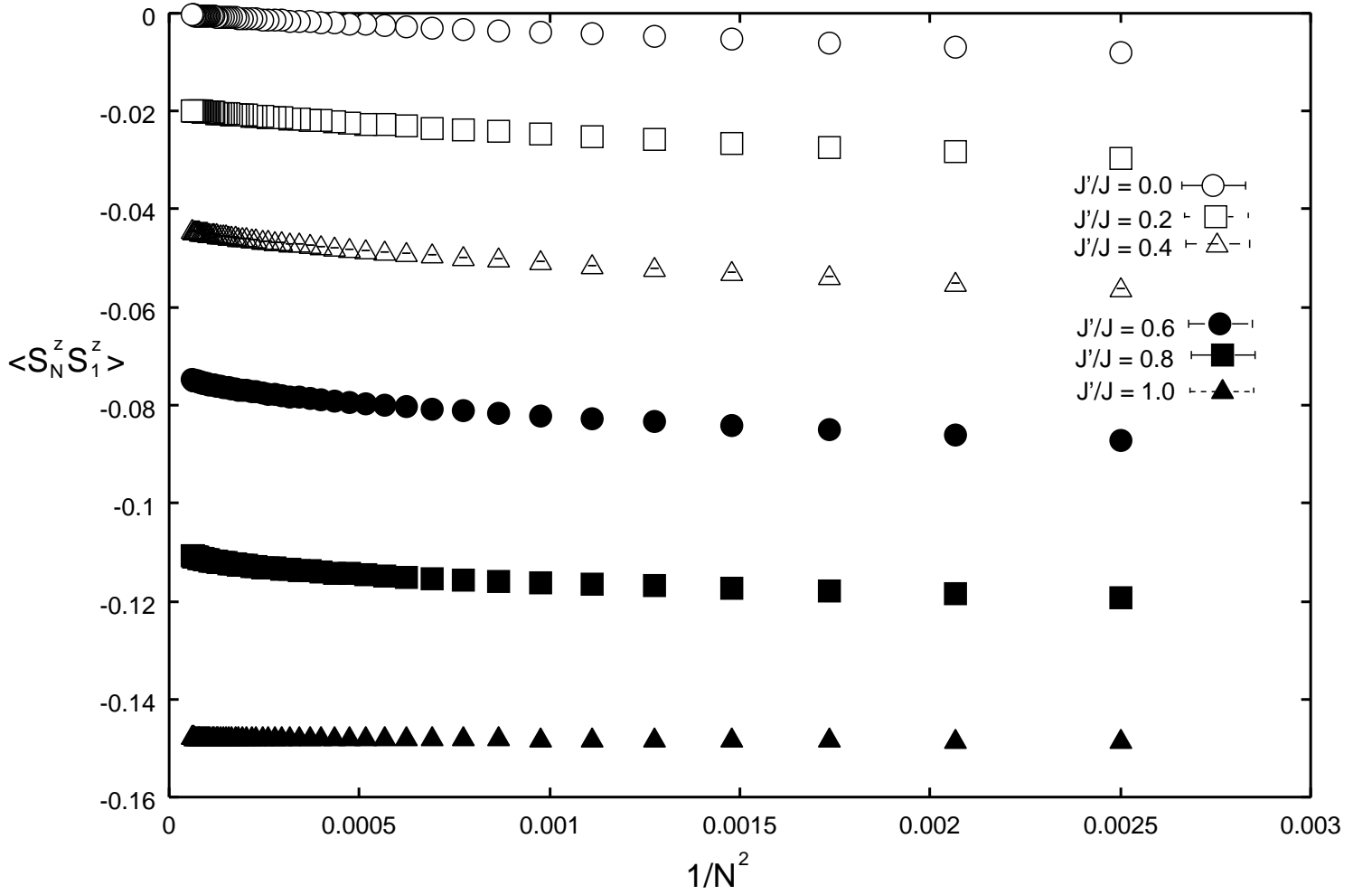


FIG. 7. The correlation  $\langle S_N^z S_1^z \rangle$  across the weak link as a function of  $1/N^2$ .